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Education

Biochemistry, Ph.D

December 2001

Department of Biochemistry and Molecular Biology, Michigan State University, East Lansing, MI.
Thesis Title: *Computational Techniques for Modeling Protein-Ligand Interactions and their Application to Serine Proteases and Asparaginyl-tRNA Synthetase*
Research Advisor: Dr. Leslie A. Kuhn
Focus: Computational methods for protein structural analysis, computational ligand screening, molecular modeling, algorithm development, protein-water interactions.

Biochemistry, B.S.

May 1996

Department of Biochemistry, Michigan State University, East Lansing, MI.
Also a member of the Honors College

Professional Experience

Senior Scientist, Drug Discovery Applications

April 2004 – October 2008

Schrödinger, Inc.,

New York, NY

Responsible for working with outside research groups in academic institutions, biotechnology companies, and pharmaceutical companies to apply the scientifically leading Schrödinger suite of drug discovery software to drug development projects, including lead identification and lead optimization. Involved use of virtual screening, pharmacophore search, QSAR, and cheminformatics methods. Had contacts with many scientists including biologists, medicinal chemists, structural biologists, and molecular modelers. Deeply involved in internal drug discovery and software validation projects involving a large amount of structural and published activity data collation as well as identifying a large number of new protein targets to greatly expand our validation suite. Involved in the design of the actual database to store this data and to make it readily accessible for other users within Schrödinger. Extensive use of the Schrödinger Python application environment for both small scale and large scale script development, including projects customized for specific Schrödinger customers. Had numerous contacts with members of various software development groups to apply my knowledge of drug discovery and knowledge from working with project collaborators to improve Schrödinger software products.

Postdoctoral Research Associate

January 2002 – March 2004

AG Klebe, Institute for Pharmaceutical Chemistry, University of Marburg

Marburg, Germany

Worked in a varied academic pharmaceutical research group predominantly on developing improved scoring functions for structure-based docking applications. This involved extensive scientific research as well as programming to implement these techniques. This project was undertaken as part of the Scoring Function Consortium, which involved steady contact with representatives from a number of major pharmaceutical companies including incorporating their suggestions into the research and giving regular progress reports. Involved in advising more junior members of the research group on their projects.

Graduate Research Assistant

Department of Biochemistry and Molecular Biology, Michigan State University

August 1996 – January 2002

East Lansing, MI

Conducted studies into methods for computational ligand screening including the use of ligand flexibility, protein side-chain flexibility, and water molecule interactions as the SLIDE docking algorithm. Developed techniques for analysis of conserved water sites in protein structures and studied such in thrombin and trypsin structures. Constructed a theoretical model of a portion of *Drosophila melanogaster* mitochondrial DNA polymerase accessory subunit that led to a proposed mode of action. Developed techniques for prediction of water molecule displacement upon ligand binding involving evolutionary computational techniques.

Lab Technician

Quality Control Department, Neogen Corporation

June, 1995 – August, 1995

Lansing, MI

I performed preliminary, final, and post-release testing on ELISA based mycotoxin detection kits. I performed analysis of customer submitted samples for mycotoxins.

Technical Competencies

Extensive knowledge of the Schrödinger suite (Maestro, Glide, MacroModel, Phase, Prime, Canvas) of molecular modeling and computational chemistry software.

Additional experience with Accelrys (InsightII), Tripos, and MOE software packages.

Extensive knowledge of the Python programming language including GUI (TKinter) programming as well as knowledge of C/C++, Perl, and shell scripting languages.

Knowledge of HTML, PHP, and MySQL web development environments.

Extensive knowledge of Windows, Linux, and Unix environments.

Publications

- M. I. Zavodsky, P. C. Sanschagrín, R. S. Korde, and L. A. Kuhn (2002) "Distilling the Essential Features of a Protein Surface for Improving Protein-Ligand Docking, Scoring, and Virtual Screening", *J. Comput. Aided. Mol. Des.*, **16**, 883–902. (co-first author)
- P. C. Sanschagrín and L. A. Kuhn (1998) "Cluster Analysis of Consensus Water Sites in Thrombin and Trypsin Shows Conservation Between Serine Proteases and Contributions to Ligand Specificity", *Protein Sci.*, **7**, 2054–2064.
- M. Podvinec, S. Pheng Lim, M. Scarsi, P. Sanschagrín, T. Schmidt, P. Shenkin, T. Schwede (2008) "Novel Inhibitors of Dengue Virus NS5 Methyltransferase: Discovery by in vitro-driven virtual screening on a PC Grid". (in preparation)
- C. A. Sotriffer, P. Sanschagrín, H. Matter, G. Klebe (2008) "SFCSScore: Scoring Functions for Affinity Prediction of Protein-Ligand Complexes", *Proteins*, **73**, 395–419.
- S. Rao, P. C. Sanschagrín, J. R. Greenwood, M. P. Repasky, W. Sherman, R. Farid (2008) "Improving Database Enrichment through Ensemble Docking", *J. Comput. Aided. Mol. Des.*, **22**, 621–627.
- R. A. Friesner, R. B. Murphy, M. P. Repasky, L. L. Frye, J. R. Greenwood, T. A. Halgren, P. C. Sanschagrín, and D. T. Mainz (2006) "Extra Precision Glide: Docking and Scoring Incorporating a Model of Hydrophobic Enclosure for Protein-ligand Complexes", *J. Med. Chem.*, **49**, 6177–6196.
- P. Block, J. Paern, E. Hüllermeier, P. Sanschagrín, C. A. Sotriffer, and G. Klebe (2006) "Physicochemical Descriptors to Discriminate Protein-Protein Interactions in Permanent and Transient Complexes Selected by Means of Machine Learning Algorithms", *Proteins*, **65**, 607–622.

- L. Fan, P. C. Sanschagrín, L. S. Kaguni, and L. A. Kuhn (1999) “The Accessory Subunit of Mitochondrial DNA Polymerase Shares Structural Homology with a Domain in Aminoacyl tRNA Synthetases: Implications for a Dual Role as a Primer Recognition Factor and Processivity Clamp”, *Proc. Natl. Acad. Sci. USA* **96**, 9527–9532.
- L. Craig, P. C. Sanschagrín, A. Rozek, S. Lackie, L. A. Kuhn, and J. K. Scott (1998) “The Role of Structure in Antibody Cross-Reactivity Between Peptides and Folded Proteins”, *J. Mol. Biol.*, **281**, 183–201.
- M. L. Raymer, W. F. Punch, E. D. Goodman, P. C. Sanschagrín, and L. A. Kuhn (1997) “Simultaneous Feature Scaling and Selection Using a Genetic Algorithm”, in *Proceedings of the Seventh International Conference on Genetic Algorithms* (T. Bäck, ed.), Morgan Kaufmann Publishers, San Francisco, pp. 561–567.
- M. L. Raymer, P.C. Sanschagrín, W. F. Punch, S. Venkataraman, E. D. Goodman, and L. A. Kuhn (1997) “Predicting Conserved Water-Mediated and Polar Ligand Interactions in Proteins Using a K-nearest-neighbors Genetic Algorithm”, *J. Mol. Biol.*, **265**, 445–464.

Presentations

- P. C. Sanschagrín, “Virtual Screening to Identify Novel Dengue Virus Inhibitors”, *American Chemical Society Fall 2008 National Meeting*, Philadelphia, Pennsylvania, August, 2008.
- P. C. Sanschagrín, S. N. Rao, J. R. Greenwood, W. Sherman, R. Farid, L. L. Frye, “Using Structural Ensembles to Improve Cross-Docking and Virtual Screening”, *International Workshop New Approaches in Drug Design & Discovery: Merging Chemical & Biological Space*, Rauschholzhausen, Germany, March 2007.
- P. C. Sanschagrín, M. I. Zavodszky, and L. A. Kuhn, “Modeling of Hydrophobic Interactions in Computational Ligand Screening: A Template Matching Approach”, *International Workshop New Approaches in Drug Design & Discovery: What Makes a Drug Attractive for its Receptor: ADMET, Affinity and Selectivity*, Rauschholzhausen, Germany, March 2001.
- P. C. Sanschagrín, M. I. Zavodszky, and L. A. Kuhn, “Template-Based Computational Screening for Ligands Including Side-chain Flexibility and Interfacial Solvent”, *Intelligent Systems for Molecular Biology*, San Diego, California, August 2000.
- P. C. Sanschagrín, L. Fan, L. S. Kaguni, and L. A. Kuhn, “Threading and Structural Analysis of a Novel DNA Polymerase Subunit Indicates Roles in Primer Recognition and Processivity”, *Thirteenth Symposium of the Protein Society*, Boston, Massachusetts, July 1999.
- P. C. Sanschagrín and L. A. Kuhn, “The Contributions of Conserved Bound Water Molecules to Thrombin and Trypsin Structure and Specificity”, *the Cardiovascular Research Forum*, American Heart Association, Michigan Affiliate, Detroit, Michigan, October 1998.
- P. C. Sanschagrín, M. L. Raymer, and L. A. Kuhn (1997) “Cluster Analysis of Multiple Serine Protease Structures Identifies Conserved Water Sites Involved in Structure and Specificity”, *West Coast Protein Crystallography Workshop*, Pacific Grove, California, March 1997.